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                                                       ENTRY     SESSION
FULL ESTIMATED COST                                     0.21        0.21

FILE 'CAPLUS' ENTERED AT 12:35:58 ON 21 NOV 2004
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FILE COVERS 1907 - 21 Nov 2004  VOL 141 ISS 22
FILE LAST UPDATED: 19 Nov 2004  (20041119/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=>
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L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
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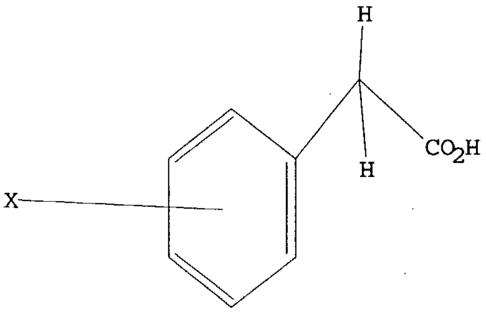

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Structure attributes must be viewed using STN Express query preparation.


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Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.





SAMPLE SEARCH INITIATED 12:36:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   5798 TO ITERATE

 17.2% PROCESSED    1000 ITERATIONS                          13 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
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PROJECTED ITERATIONS:       111395 TO   120525
PROJECTED ANSWERS:             987 TO     2027

L2           13 SEA SSS SAM L1



L3          13 L2

=> l3  and malonate
L3 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
'HELP COMMANDS" at an arrow prompt (=>).

=> s l3 and malonate
         22929 MALONATE
L4           3 L3 AND MALONATE

=> d 1-3 ibib abs hitstr

L4   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:951003  CAPLUS
DOCUMENT NUMBER:          140:16723
TITLE:                    Preparation of 1,2-azole derivatives with hypoglycemic
                          and hypolipidemic activity
INVENTOR(S):              Maekawa, Tsuyoshi; Hara, Ryoma; Odaka, Hiroyuki;
                          Kimura, Hiroyuki; Mizufune, Hideya; Fukatsu, Kohji
PATENT ASSIGNEE(S):       Takeda Chemical Industries, Ltd., Japan
SOURCE:                   PCT Int. Appl., 564 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE         APPLICATION NO.        DATE
     ---------------     ----   --------     --------------------   --------
     WO 2003099793        A1    20031204     WO 2003-JP6389         20030522
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     JP 2004277397        A2    20041007     JP 2003-144984         20030522
PRIORITY APPLN. INFO.:                       JP 2002-151405      A  20020524
                                             JP 2002-287161      A  20020930
                                             JP 2003-16748       A  20030124

OTHER SOURCE(S):          MARPAT 140:16723
GI
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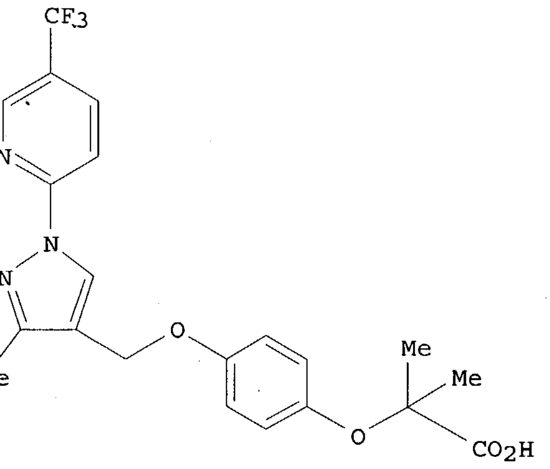


I

B 1,2-Azole derivs. A-B-Xa-Ya-Xb-Yb-C-Xc-Yc-C(:O)-R (I; e.g. II) wherein ring A optionally has 1-3 substituents; ring B is a 1,2-azole ring which may further have 1 to 3 substituents; Xa, Xb and Xc are the same or different and each is a bond, -O-, -S- and the like; Ya is a divalent aliphatic hydrocarbon residue having 1-20 C atoms; Yb and Yc are the same or different and each is a bond or a divalent aliphatic hydrocarbon residue having 1-20 C atoms; ring C is a monocyclic aromatic ring which may further have 1 to 3 substituents; and R = -OR4 (R4 is H atom or (un)substituted hydrocarbon group) and the like, or a salt thereof or a prodrug thereof is useful as an agent for the prophylaxis or treatment of diabetes and the like. Hypoglycemic and hypolipidemic actions in mice are tabulated for about 50 examples of I; e.g. a 53 % rate of decrease in blood glucose level in the presence of 0.005 % [2-[3-[3-isopropyl-1-[5-(trifluoromethyl)-2-pyridinyl]-1H-pyrazol-4-yl]propoxy]-3-methylphenyl]acetic acid and a 77 % rate of decrease in blood triglyceride level in the presence of 0.005 % 2-methyl-2-[4-[3-methyl-1-[5-(trifluoromethyl)-2-pyridyl]-1H-pyrazol-4-ylmethoxy]phenoxy]propionic acid when the level (glucose or triglyceride) of the non-treated group is taken as 100 %. Plasma anti-arteriosclerosis index-enhancing action in mice is tabulated for 34 examples of I, e.g. 25 % for [3-methoxy-2-[3-[3-propyl-1-[5-(trifluoromethyl)-2-pyridyl]-1H-pyrazol-4-yl]propoxy]phenyl]acetic acid. PPARγ-RXRα and PPARδ-RXRα heterodimer ligand activity is tabulated for 59 and 80 examples, resp., of I, e.g. EC50 = 3.8 nM for PPARγ-RXRα for [2-[3-[3-cyclohexyl-1-[5-(trifluoromethyl)-2-pyridinyl]-1H-pyrazol-4-yl]propoxy]-3-methylphenyl]acetic acid. Nearly 400 example prepns. of I and 351 example prepns. of intermediates are included. For example, [4-[3-[3-[4-(trifluoromethyl)phenyl]-5-isoxazolyl]propoxy]phenyl]acetic acid was obtained in 25 % yield from a mixture of 3-[3-[4-(trifluoromethyl)phenyl]-5-isoxazolyl]-1-Pr methanesulfonate, NaI, Me 2-(4-hydroxyphenyl)acetate, K2CO3 and DMF; details of the preparation of the mesylate are also given.

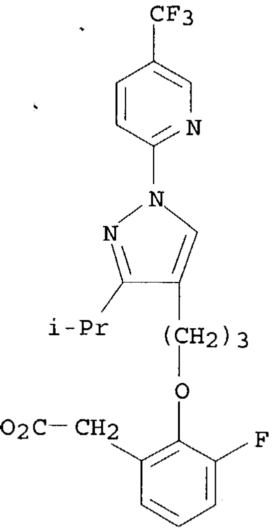
T **628334-96-3P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of 1,2-azole derivs. with hypoglycemic and hypolipidemic activity)

N 628334-96-3 CAPLUS

N Benzeneacetic acid, 3-fluoro-2-[3-[3-(1-methylethyl)-1-[5-(trifluoromethyl)-2-pyridinyl]-1H-pyrazol-4-yl]propoxy]- (9CI) (CA INDEX NAME)



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EFERENCE COUNT:          19    THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

4   ANSWER 2 OF 3  CAPLUS  COPYRIGHT 2004 ACS on STN
CCESSION NUMBER:         2001:935563  CAPLUS
OCUMENT NUMBER:          136:54021
ITLE:                    Thyroid receptor ligands, namely 3,5-dichloro-4-(3-
                         bromo-4-amidophenoxy)phenylacetic acids and analogs,
                         pharmaceutical compositions comprising them, and their
                         use in the treatment of disorders influenced by
                         thyroid hormones
NVENTOR(S):              Li, Yi-Lin; Malm, Johan; Litten, Chris; Garcia
                         Collazo, Ana Maria; Garg, Neeraj
ATENT ASSIGNEE(S):       Karo Bio AB, Swed.
OURCE:                   PCT Int. Appl., 86 pp.
                         CODEN: PIXXD2
OCUMENT TYPE:            Patent
ANGUAGE:                 English
AMILY ACC. NUM. COUNT:   1
ATENT INFORMATION:

    PATENT NO.           KIND   DATE         APPLICATION NO.        DATE
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    WO 2001098256         A1    20011227     WO 2001-EP6815         20010615
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
            RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
            UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    EP 1296936            A1    20030402     EP 2001-951600         20010615
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    JP 2004501132         T2    20040115     JP 2002-504212         20010615
    US 2004097589         A1    20040520     US 2003-311524         20030422
RIORITY APPLN. INFO.:                        GB 2000-15205      A   20000621
                                             WO 2001-EP6815     W   20010615
THER SOURCE(S):          MARPAT 136:54021
I
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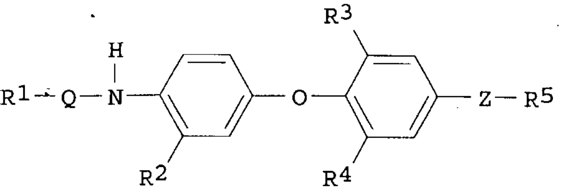

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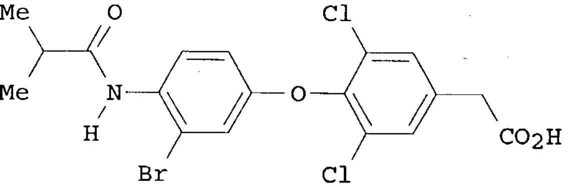


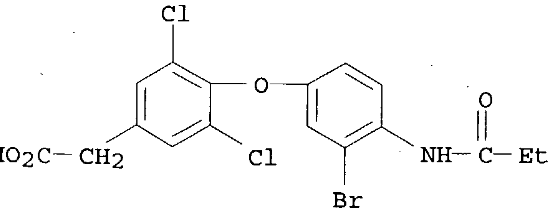
II

AB The invention relates to compds. I or pharmaceutically acceptable salts thereof [wherein: R1 = (un)substituted aryl, heteroaryl, alk(en/yn)yl, cycloalkyl; R2 = H, halo, NO2, CN, aryl, heteroaryl, alk(en/yn)yl, cycloalkyl; R1 can be linked to R2, thus forming an (un)substituted aza-containing C5-8 heterocyclic ring; Q = CO, SO, SO2, NHCS, or NHCO; R3, R4 = halo, (un)substituted alk(en/yn)yl, cycloalkyl, or bioisosteric equivalent; Z = (CH2)n, CH:CH, O(CH2)m, or NH(CH2)m; n = 0, 1, 2, or 3; m = 1 or 2; R5 = CO2H, PO(OH)2, PO(OH)NH2, SO2OH, CONHOH, NHCOCO2H, NHCOCH2CO2H, CONHSO2R', or CONR'R'' (R' and R'' not explicitly defined) where the amine portion is derived from an L- or D-amino acid or a mixture; or any other possible bioisosteric equivalent of all the groups above; including all stereoisomers, and prodrug esters]. Also disclosed are methods of preparing I, and methods for using them, such as in the regulation of metabolism I are thyroid receptor ligands, and are preferably selective for the thyroid hormone receptor β. Over 80 examples are given. For instance, 3,5-dichloro-4-(3-bromo-4-isobutyramidophenoxy)phenylacetic acid (II) was prepared in 9 steps as follows: (1) bromination of 2,6-dichlorophenol in the 4-position (85%), (2) etherification with 4-fluoronitrobenzene (45%), (3) coupling of the bromide with HC.tplbond.CSiMe3 (53%), (4) desilylation and oxidation to an acid, (5) conversion to the Me ester, (6) hydrogenation of the nitro group, (7) ring bromination adjacent to amino (57%), (8) amidation of the amino group with isobutyryl chloride (40%), and (9) alkaline hydrolysis of the ester (82%). Compds. I of the examples bound to thyroid receptor β with IC50 values of 0.2 nM to 10,000 nM.

IT **383181-88-2P**, [3,5-Dichloro-4-[3-bromo-4-(propanoylamino)phenoxy]phenyl]acetic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of dichloro(bromoamidophenoxy)phenylacetic acids and analogs as thyroid hormone receptor ligands)

RN 383181-88-2 CAPLUS

CN Benzeneacetic acid, 4-[3-bromo-4-[(1-oxopropyl)amino]phenoxy]-3,5-dichloro- (9CI) (CA INDEX NAME)



EFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

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                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4   ANSWER 3 OF 3  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1992:407943  CAPLUS
DOCUMENT NUMBER:          117:7943
TITLE:                    Preparation of pyrido[3,2,1-ij]cinnoline-8-
                          carboxylates as antimicrobial agents
INVENTOR(S):              Yokomoto, Masaharu; Yazaki, Akira; Hayashi, Norihiro;
                          Hatono, Shunso; Inoue, Satoshi; Kuramoto, Yasuhiro
PATENT ASSIGNEE(S):       Wakunaga Pharmaceutical Co., Ltd., Japan; Fujisawa
                          Pharmaceutical Co., Ltd.
SOURCE:                   Eur. Pat. Appl., 90 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.          KIND   DATE         APPLICATION NO.         DATE
     ---------------     ----   --------     --------------------    --------
     EP 470578            A1    19920212     EP 1991-113212          19910806
     EP 470578            B1    19961106
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
     AU 9181630           A1    19920213     AU 1991-81630           19910805
     CA 2048511           AA    19920210     CA 1991-2048511         19910806
     AT 144983            E     19961115     AT 1991-113212          19910806
     US 5254685           A     19931019     US 1991-741333          19910807
     FI 9103769           A     19920210     FI 1991-3769            19910808
     NO 9103087           A     19920210     NO 1991-3087            19910808
     HU 59139             A2    19920428     HU 1991-2649            19910808
     ZA 9106268           A     19920429     ZA 1991-6268            19910808
     CN 1059144           A     19920304     CN 1991-105462          19910809
     JP 05059052          A2    19930309     JP 1991-200673          19910809
     US 5399553           A     19950321     US 1993-76938           19930616
PRIORITY APPLN. INFO.:                       JP 1990-211190      A   19900809
                                             JP 1991-80144       A   19910412
                                             JP 1991-164356      A   19910704
                                             US 1991-741333      A2  19910807
                                             US 1991-789071      B1  19911107
OTHER SOURCE(S):          MARPAT 117:7943
GI
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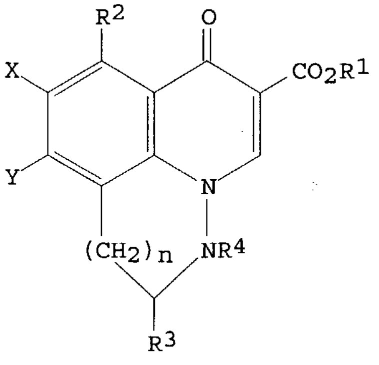

I

AB Title compds. I (R1 = H, carboxyl protecting group; R2 = H, halo, amino or protected amino group; R3 = H, alkyl; R4 = H, (substituted)alkyl, acyl, aralkyl; X = H, halo; Y = halo, H2N, HO, cycloalkyl-, mono-, dialkylamino, (substituted)cyclic amino, (substituted)alkyl (substituted) cycloalkenyl, etc.; n = 0-2) and a salt thereof, are prepared I (R1 = R2 = R3 = H, R4 = Me, X = Y = F, n = 1) (preparation given), cis-(-)-3-amino-4-methylpyrrolidine-2HCl, and 1,8-diazabicyclo[5.4.0]-7-undecene were added to DMF, to give after workup I (R1 = R2 = R3 = H, R4 = Me, X = F, Y = cis-(-)-3-amino-4-

```
     methylpyrrolidin-1-yl, n = 1) (II).  The min. inhibitory concentration of II
     against Escherichia coli, Staphycoccus aureus, and Pseudomonas aeruginosa
     was 0.025, 0.1 and 0.2 µg/mL, resp.
IT   141449-35-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, as antimicrobial)
RN   141449-35-6  CAPLUS
CN   1H,7H-Pyrido[3,2,1-ij]cinnoline-4-acetic acid, 8-carboxy-5-fluoro-2,3-
     dihydro-1-methyl-7-oxo- (9CI)  (CA INDEX NAME)
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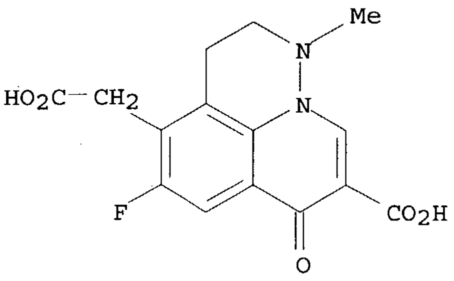

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=> s l1 full
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Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 12:38:18 FILE 'REGISTRY'
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100.0% PROCESSED  114921 ITERATIONS                         2651 ANSWERS
SEARCH TIME: 00.00.01

L5          2651 SEA SSS FUL L1



L6         4982 L5

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         22929 MALONATE
L7          170 L6 AND MALONATE

=> s l6 and malonate and decarboxyl?
         22929 MALONATE
         61273 DECARBOXYL?
L8           29 L6 AND MALONATE AND DECARBOXYL?

=> s l8 and py<2002
      21585351 PY<2002
L9           25 L8 AND PY<2002

=> d 1-25 ibib abs hitstr

L9   ANSWER 1 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2000:828893  CAPLUS
DOCUMENT NUMBER:          134:4768
TITLE:                    Preparation of phthalonitriles
INVENTOR(S):              Ikeno, Ikuyo
PATENT ASSIGNEE(S):       Nippon Shokubai Kagaku Kogyo Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 6 pp.
                          CODEN: JKXXAF
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DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000327652	A2	20001128	JP 1999-136706	19990518 <--

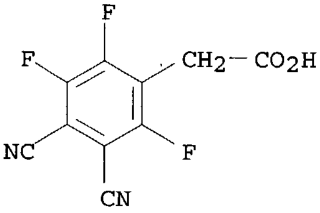
PRIORITY APPLN. INFO.: JP 1999-136706 19990518
OTHER SOURCE(S): CASREACT 134:4768; MARPAT 134:4768
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

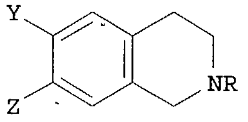
AB Title compds. I (X1-X3 = H, halo, alkyl, alkoxy) are prepared by reaction of fluorophthalonitriles II (X1-X3 = same as I) with CH2R1R2 (R1, R2 = cyano, CO2R3; R3 = alkyl) in the presence of basic compds. and reaction of phthalonitriles III (X1-X3, R1, R2 = same as above) in the presence of acid catalysts. 3,4,5,6-Tetrafluorophthalonitrile (19.998 g) was reacted with di-Et **malonate** in DMF in the presence of K2CO3 at 60° for 6 h to give 32.454 g di-Et 2-(3,4-dicyano-2,5,6-trifluorophenyl)**malonate**, which (10.121 g) was hydrolyzed with HCl in AcOH at 103° for 3 h to give 4.539 g 2-(3,4-dicyano-2,5,6-trifluorophenyl)acetic acid.

IT **308803-65-8P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of phthalonitriles by condensation of fluorophthalonitriles with malonates and **decarboxylation**)

RN 308803-65-8 CAPLUS
CN Benzeneacetic acid, 3,4-dicyano-2,5,6-trifluoro- (9CI) (CA INDEX NAME)



L9 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:325272 CAPLUS
DOCUMENT NUMBER: 129:16037
TITLE: Synthesis of 1,2,3,4-Tetrahydroisoquinolines Containing Electron-Withdrawing Groups
AUTHOR(S): Quallich, George J.; Makowski, Teresa W.; Sanders, Andrew F.; Urban, Frank J.; Vazquez, Enrique
CORPORATE SOURCE: Process Research and Development Central Research Division, Pfizer Inc., Groton, CT, 06340, USA
SOURCE: Journal of Organic Chemistry (**1998**), 63(12), 4116-4119
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:16037
GI



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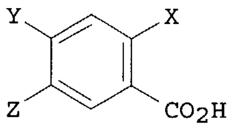
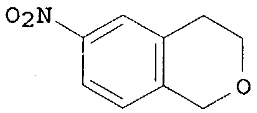


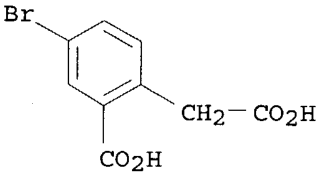
II



III

AB A general method to prepare 1,2,3,4-tetrahydroisoquinolines and isochromans containing electron withdrawing groups in the aromatic ring is detailed. Tetrahydroisoquinolines I (Y = H, NO2; Z = H, Br, CF3; R = H, H2C:CHCH2, Ph) were prepared from halobenzoic acids II (X = Br, Cl; Y= H, NO2; Z = H, Br, CF3) by a sequence using a copper-catalyzed coupling with di-Me **malonate**, acid hydrolysis and **decarboxylation**, borane reduction, mesylate formation, and displacement with RNH2 (R = H, H2C:CHCH2, Ph). Isochroman III was prepared in one step by a Mitsunobu displacement of a diol intermediate in the preparation of I. Sodium methoxide was found to be a useful base for the copper (I) bromide-catalyzed coupling of di-Me **malonate** with II. Closure of the tetrahydroisoquinoline ring system was studied using mesylates and chlorides as leaving groups, and various amines RNH2 (R = H, Me3Si, H2C:CHCH2, Ph) as nucleophiles; the cyclization proceeded best with mesylate as the leaving group and either aniline or allylamine at 25° and 1 atm, or NH3 at 120 atmospheric

IT **19725-82-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrahydroisoquinolines and isochromans with electron-withdrawing groups)
RN 19725-82-7 CAPLUS
CN Benzeneacetic acid, 4-bromo-2-carboxy- (9CI) (CA INDEX NAME)

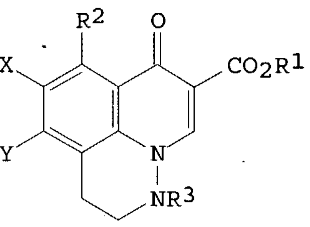


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:579602 CAPLUS
DOCUMENT NUMBER: 121:179602
TITLE: Preparation of pyrido[3.2.1-ij]cinnolines and microbicides containing them
INVENTOR(S): Inoe, Satoshi; Yoshida, Jiro; Yokomoto, Masaharu; Yazaki, Akira; Hayashi, Norihiro; Amano, Hirotaka
PATENT ASSIGNEE(S): Wakunaga Seiyaku Kk, Japan; Fujisawa Pharmaceutical Co
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05279364	A2	19931026	JP 1993-16527	19930203 <--
PRIORITY APPLN. INFO.:			JP 1992-22704	19920207

OTHER SOURCE(S): MARPAT 121:179602
GI



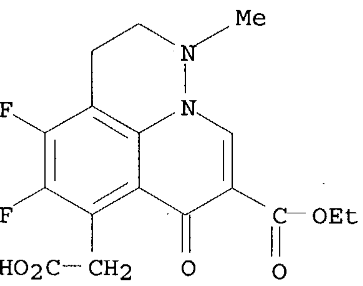
I

AB The title compds. I [R1 = H, protective group; R2 = (substituted) lower alkyl, (protected) OH, NO2; R3 = (substituted) lower alkyl; X = halo; Y = halo, (substituted) cyclic amino] are prepared as microbicides. A toluene solution of 1.31 g tert-Bu **malonate** was treated with NaH at room temperature for 30 min, mixed with 450 mg I (R1 = Et, R2 = X = Y = F, R3 = Me) (preparation given), and stirred at room temperature for 30 min to give 220 mg I [R1 = Et, R2 = CH(CO2CMe3)2, X = Y = F, R3 = Me]. I.HCl [R1 = H, R2 = R3 = Me, X = F, Y = cis-(-)-3-amino-4-methylpyrrolidin-1-yl] had MIC of 0.05 μg/mL in vitro against Escherichia coli NIH JC-2 (IFO 12734).

IT **155621-77-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as microbicide)

RN 155621-77-5 CAPLUS

CN 1H,7H-Pyrido[3,2,1-ij]cinnoline-6-acetic acid, 8-(ethoxycarbonyl)-4,5-difluoro-2,3-dihydro-1-methyl-7-oxo- (9CI) (CA INDEX NAME)

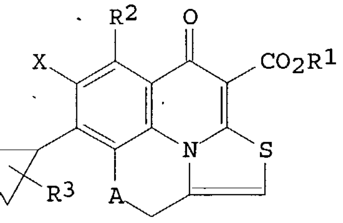


L9 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:185471 CAPLUS
DOCUMENT NUMBER: 114:185471
TITLE: Preparation of 1,9-bridged 8-cyclopropyl-5-oxo-5H-thiazolo[3,2-a]quinoline-4-carboxylic acids as broad-spectrum bactericides
INVENTOR(S): Narita, Hirokazu; Todo, Yozo; Takagi, Hiroyasu; Iino, Fumihiko; Myajima, Mikako; Fukuoka, Yoshikazu
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02286686	A2	19901126	JP 1989-108431	19890427 <--
JP 2787704	B2	19980820		

PRIORITY APPLN. INFO.: JP 1989-108431 19890427
OTHER SOURCE(S): MARPAT 114:185471
GI



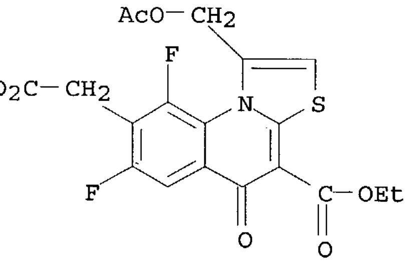
I

3 The title compds. [I; R1 = H, carboxy-protective group; R2 = H, halo, alkoxy, (un)protected hydroxy, (un)protected amino, (un)protected lower alkylamino, di(lower alkyl)amino; R3 = H, lower alkyl, (un)protected amino, (un)protected lower alkylamino, di(lower alkyl)amino, (un)protected carboxy, (un)protected lower aminoalkyl, (un)protected lower alkylaminoalkyl, (un)protected lower hydroxyalkyl; A = O, S, (lower alkyl)imino; X = halo] and their salts were prepared Et 1-acetoxymethyl-8-cyclopropyl-7,9-difluoro-5-oxo-5H-thiazolo[3,2-a]quinoline-4-carboxylate (preparation given) in EtOH was treated with EtONa at room temperature for 1 h to give I (R1 = Et, R2 = R3 = H, A = O, X = F), which in EtOH/dioxane was treated with an aqueous NaOH solution at 40° for 1.5 h to give 90.4% I (R1 = R2 = R3 = H, A = O, X = F) (II). Min. inhibitory concentration of II on Staphylococcus aureus F-597 and Escherichia coli NIHJ were 0.05 and ≤0.025 µg/mL, resp.

T **133369-03-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and protection of, with diphenyldiazomethane, benzhydryl ester from)

J 133369-03-6 CAPLUS

J 5H-Thiazolo[3,2-a]quinoline-8-acetic acid, 1-[(acetyloxy)methyl]-4-(ethoxycarbonyl)-7,9-difluoro-5-oxo- (9CI) (CA INDEX NAME)



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9   ANSWER 5 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
CCESSION NUMBER:         1991:163770  CAPLUS
OCUMENT NUMBER:          114:163770
ITLE:                    Preparation of alkylhalobenzene derivatives
NVENTOR(S):              Marhold, Albrecht; Fischer, Reiner
ATENT ASSIGNEE(S):       Bayer A.-G., Germany
OURCE:                   Ger. Offen., 9 pp.
                         CODEN: GWXXBX
OCUMENT TYPE:            Patent
ANGUAGE:                 German
AMILY ACC. NUM. COUNT:   1
ATENT INFORMATION:

    PATENT NO.           KIND   DATE       APPLICATION NO.        DATE
    ---------------      ----   --------   --------------------   --------
    DE 3909213            A1    19901011   DE 1989-3909213        19890321 <--
    EP 394644             A2    19901031   EP 1990-104397         19900308 <--
    EP 394644             A3    19910116
    EP 394644             B1    19941005
        R:  BE, CH, DE, FR, GB, IT, LI
    JP 02279641           A2    19901115   JP 1990-62828          19900315 <--
    JP 2744669            B2    19980428
IORITY APPLN. INFO.:                       DE 1989-3909213        19890321
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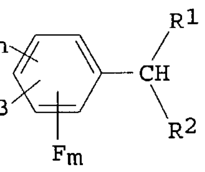
HER SOURCE(S):   MARPAT 114:163770



I

Halobenzene derivs. I (R1 = H, CO2R4; R2 = cyano, CO2R4 or CO2H, H, cyano when R1 = H; R3 = H, cyano, Me, CF3, Cl, CHR1R2; R4 = C1-4 alkyl; m = 0-4; n = 0-3 and 2 ≤ m + n ≤ 4 excluding the combination m = 4, n = 0, and R3 = CF3) were prepared For example, a mixture of 1,3-dichlorotetrafluorobenzene, K2CO3, and NCCH2CO2Me in dry DMF was heated 10 h at 120°. The solvent was removed and the residue was acidified to give Me 2-(2,4-dichlorotrifluorophenyl)cyanoacetate. Subsequent hydrolysis and **decarboxylation** gave I (R1 = H, R2 = CO2H).

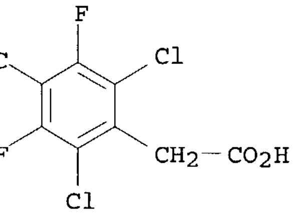
132992-22-4P 132992-23-5P 132992-28-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and **decarboxylation** of)

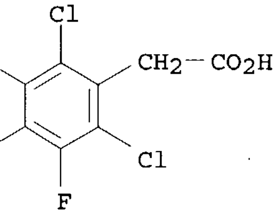
132992-22-4 CAPLUS

Benzeneacetic acid, 2,6-dichloro-3,5-difluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



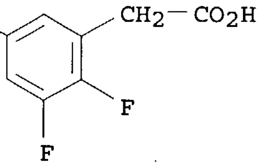
132992-23-5 CAPLUS

Benzeneacetic acid, 2,4,6-trichloro-3,5-difluoro- (9CI) (CA INDEX NAME)



132992-28-0 CAPLUS

Benzeneacetic acid, 2,3,5-trifluoro- (9CI) (CA INDEX NAME)



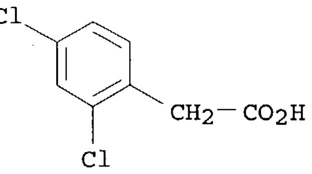
19719-28-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and hydrodechlorination of)

RN 19719-28-9 CAPLUS

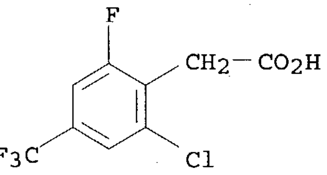
CN Benzeneacetic acid, 2,4-dichloro- (9CI) (CA INDEX NAME)



IT **132992-24-6P 132992-25-7P 132992-26-8P**
132992-27-9P 132992-34-8P 132992-36-0P,
4-Trifluoromethyl-2,6-dichlorophenylacetic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

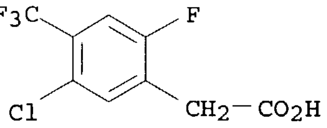
RN 132992-24-6 CAPLUS

CN Benzeneacetic acid, 2-chloro-6-fluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



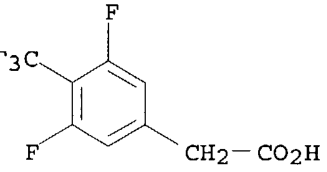
RN 132992-25-7 CAPLUS

CN Benzeneacetic acid, 5-chloro-2-fluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



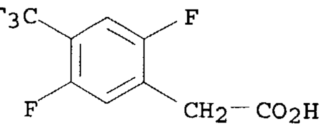
RN 132992-26-8 CAPLUS

CN Benzeneacetic acid, 3,5-difluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 132992-27-9 CAPLUS

CN Benzeneacetic acid, 2,5-difluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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RN   132992-34-8  CAPLUS
CN   Benzeneacetic acid, 3,4,6-trifluoro-2-(trifluoromethyl)- (9CI)  (CA INDEX
     NAME)
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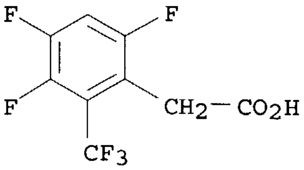

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RN   132992-36-0  CAPLUS
CN   Benzeneacetic acid, 2,6-dichloro-4-(trifluoromethyl)- (9CI)  (CA INDEX
     NAME)
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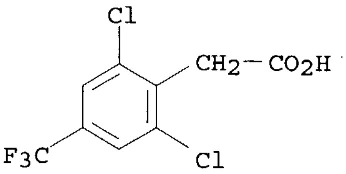

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L9   ANSWER 6 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        1990:478417  CAPLUS
DOCUMENT NUMBER:         113:78417
TITLE:                   Preparation, testing, and formulation of
                         oxopyridobenzoxazinecarboxylates, -
                         benzothiazinecarboxylates, and -
                         quinoxalinecarboxylates as antibacterials
INVENTOR(S):             Narita, Hirokazu; Todo, Yozo; Nitta, Jun; Takagi,
                         Hiroyasu; Iino, Fumihiko; Miyajima, Mikako; Fukuoka,
                         Yoshikazu; Saikawa, Isamu
PATENT ASSIGNEE(S):      Toyama Chemical Co., Ltd., Japan
SOURCE:                  Ger. Offen., 38 pp.
                         CODEN: GWXXBX
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND  DATE         APPLICATION NO.        DATE
     ---------------     ----  --------     --------------------   --------
     DE 3913245           A1   19891102     DE 1989-3913245        19890421 <--
     DE 3913245           C2   19990715
     JP 02028178          A2   19900130     JP 1989-75873          19890328 <--
     JP 05088714          B4   19931224
     GB 2217710           A1   19891101     GB 1989-8096           19890411 <--
     GB 2217710           B2   19911204
     CA 1340493           A1   19990413     CA 1989-596351         19890411 <--
     AU 8932661           A1   19891026     AU 1989-32661          19890412 <--
     AU 601324            B2   19900906
     IL 89931             A1   19930610     IL 1989-89931          19890412 <--
     US 4990508           A    19910205     US 1989-337656         19890413 <--
     DK 8901925           A    19891024     DK 1989-1925           19890420 <--
     ZA 8902906           A    19891227     ZA 1989-2906           19890420 <--
     SE 8901464           A    19891024     SE 1989-1464           19890421 <--
     SE 504625            C2   19970317
     FI 8901910           A    19891024     FI 1989-1910           19890421 <--
     FI 91529             B    19940331
     FI 91529             C    19940711
     NO 8901650           A    19891024     NO 1989-1650           19890421 <--
     NO 171214            B    19921102
     NO 171214            C    19930210
     FR 2630441           A1   19891027     FR 1989-5335           19890421 <--
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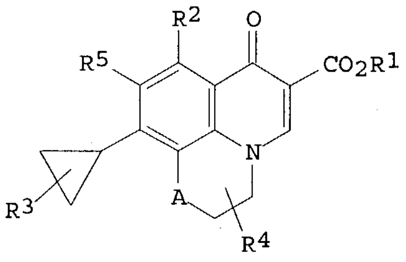
FR 2630441	B1	19941014		
NL 8901007	A	19891116	NL 1989-1007	19890421 <--
NL 192832	B	19971103		
NL 192832	C	19980304		
HU 51621	A2	19900528	HU 1989-1938	19890421 <--
HU 205759	B	19920629		
ES 2016012	A6	19901001	ES 1989-1409	19890421 <--
CH 680793	A	19921113	CH 1989-1530	19890421 <--
AT 8900959	A	19940415	AT 1989-959	19890421 <--
BE 1003252	A4	19920211	BE 1989-452	19890424 <--
JP 05043464	A2	19930223	JP 1991-359562	19911227 <--
JP 07005466	B4	19950125		
PRIORITY APPLN. INFO.:			JP 1988-100628	19880423
			JP 1989-75873	19890328

OTHER SOURCE(S): MARPAT 113:78417

GI



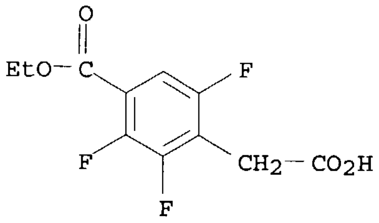
I

AB The title compds. [I; R1 = H, protecting group; R2 = H, halo, alkoxy, (protected) OH, amino; R3 = R2, (protected) CO2H, aminoalkyl, hydroxyalkyl; R4 = H, alkyl, haloalkyl, (protected) hydroxyalkyl; R4C = atoms to complete a ring; R5 = halo; A = O, S, imino], were prepared Thus, Et 2-(4-cyclopropyl-1,3,5,6-tetrafluorobenzoyl)-3-(2-hydroxy-1-methylethylamino)acrylate and K2CO3 were stirred 30 min in DMF at 80-90° to give 84.5% Et 7-cyclopropyl-5,6,8-trifluoro-1-(2-hydroxy-1-methylethyl)-1,4-dihydro-4-oxo-3-quinolinecarboxylate. The latter was stirred 15 h with NaH in DMF at 80-90° to give 39.1% Et 10-cyclopropyl-8,9-difluoro-3methyl-7-oxo-2,3-dihydro-7H-pyrido[1,2,3-de][1,4]benzoxazine-6-carboxylate. Several I showed min. inhibitory concentrate ≤0.05 µg/mL against Escherichia coli. Tablets were prepared containing S-10-1-(aminocyclopropyl)-9-fluoro-3-methyl-7-oxo-2,3-dihydro-7H-pyrido[1,2,3-de][1,4]benzoxazine-6-carboxylate.HCl.

IT **123161-38-6P**, Ethyl 4-carboxymethyl-2,3,5-trifluorobenzoate
127045-48-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antibacterial)

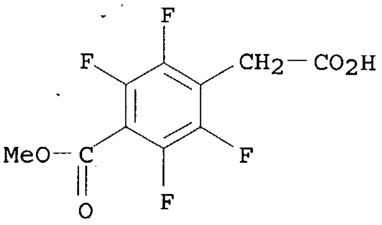
RN 123161-38-6 CAPLUS

CN Benzeneacetic acid, 4-(ethoxycarbonyl)-2,3,6-trifluoro- (9CI) (CA INDEX NAME)



RN 127045-48-1 CAPLUS

CN Benzeneacetic acid, 2,3,5,6-tetrafluoro-4-(methoxycarbonyl)- (9CI) (CA INDEX NAME)



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L9   ANSWER 7 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1990:172308  CAPLUS
DOCUMENT NUMBER:          112:172308
TITLE:                    Novel quinoline derivatives, processes for preparation
                          thereof, and antibacterial agent containing them
INVENTOR(S):              Matsumoto, Junichi; Minamida, Akira; Hirose, Tohru;
                          Nakano, Junji; Nakamura, Shinichi
PATENT ASSIGNEE(S):       Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE:                   Eur. Pat. Appl., 27 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND  DATE        APPLICATION NO.       DATE
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     EP 319906            A2   19890614    EP 1988-120345        19881206 <--
     EP 319906            A3   19900502
         R:  AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
     NO 8805426           A    19890612    NO 1988-5426          19881206 <--
     ZA 8809188           A    19890830    ZA 1988-9188          19881208 <--
     DK 8806888           A    19890612    DK 1988-6888          19881209 <--
     FI 8805722           A    19890612    FI 1988-5722          19881209 <--
     AU 8826766           A1   19890615    AU 1988-26766         19881209 <--
     CS 270600            B2   19900712    CS 1988-8172          19881209 <--
     DD 283640            A5   19901017    DD 1988-322934        19881209 <--
     CN 1034205           A    19890726    CN 1988-108598        19881210 <--
PRIORITY APPLN. INFO.:                     JP 1987-314790     A  19871211
                                           JP 1988-280610     A  19881107
OTHER SOURCE(S):          MARPAT 112:172308
GI
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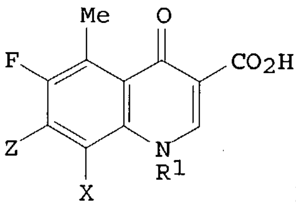

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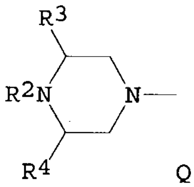
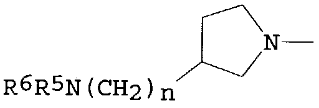


Q1



Q2

AB Quinoline derivs. [I; R1 = C1-5 alkyl, C3-6 cycloalkyl, (un)substituted Ph; X = H, halo; Z = Q1, Q2; R2-R6 = H, C1-5 alkyl; n = 0, 1], esters and salts thereof are useful for the treatment of bacterial infections. 1-Cyclopropyl-6,7,8-trifluoro-5-methyl-1,4-dihydro-4-oxoquinoline-3-carboxylic acid (preparation given) was treated with cis-2,6-dimethylpiperazine to give 1-cyclopropyl-6,8-difluoro-5-methyl-7-(cis-3,5-dimethyl-1-piperazinyl)-1,4-dihydro-4-oxoquinoline-3-carboxylic acid (II). A capsule contained II 250, starch 50, lactose 35, and talc 15 mg. II suspended in 0.4% CM-cellulose was orally administered to mice infected with Streptococcus pyogenes. The ED50 was 5.01 mg/kg. In vitro antibacterial activity, antichlamydial activity, and antimycoplasmal activity of II were detailed.

IT **126309-03-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

```
     (Reactant or reagent)
        (preparation and decarboxylation of)
RN   126309-03-3  CAPLUS
CN   1,3-Benzenedicarboxylic acid, 4-(carboxymethyl)-2,5,6-trifluoro- (9CI)
     (CA INDEX NAME)
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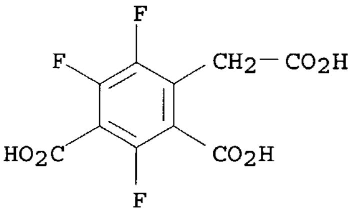

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L9   ANSWER 8 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1986:424187  CAPLUS
DOCUMENT NUMBER:          105:24187
TITLE:                    3-Substituted 2-oxindole-1-carboxamides as analgesic
                          and antiinflammatory agents
INVENTOR(S):              Kadin, Saul B.
PATENT ASSIGNEE(S):       Pfizer Inc., USA
SOURCE:                   U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 590,659,
                          abandoned.
                          CODEN: USXXAM
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.          KIND  DATE          APPLICATION NO.      DATE
     ---------------     ----  --------      --------------------  --------
     US 4556672           A    19851203      US 1984-684634        19841221 <--
     IN 162090            A    19880326      IN 1985-DE147         19850221 <--
     EP 156603            A2   19851002      EP 1985-301808        19850315 <--
     EP 156603            A3   19860212
     EP 156603            B1   19890823
         R:  AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE
     CA 1251441           A1   19890321      CA 1985-476605        19850315 <--
     AT 45731             E    19890915      AT 1985-301808        19850315 <--
     DK 8501213           A    19850920      DK 1985-1213          19850318 <--
     DK 162090            B    19910916
     DK 162090            C    19920224
     FI 8501069           A    19850920      FI 1985-1069          19850318 <--
     FI 82042             B    19900928
     FI 82042             C    19910110
     NO 8501054           A    19850920      NO 1985-1054          19850318 <--
     NO 165799            B    19910102
     NO 165799            C    19910410
     AU 8540059           A1   19850926      AU 1985-40059         19850318 <--
     AU 549927            B2   19860220
     ES 541372            A1   19851216      ES 1985-541372        19850318 <--
     HU 37398             A2   19851228      HU 1985-992           19850318 <--
     HU 196178            B    19881028
     DD 232039            A5   19860115      DD 1985-274214        19850318 <--
     ZA 8501991           A    19861126      ZA 1985-1991          19850318 <--
     IL 74631             A1   19880731      IL 1985-74631         19850318 <--
     IL 85130             A1   19880731      IL 1985-85130         19850318 <--
     SU 1445556           A3   19881215      SU 1985-3869754       19850318 <--
     PL 145951            B1   19881231      PL 1985-252434        19850318 <--
     JP 60209564          A2   19851022      JP 1985-55627         19850319 <--
     JP 04037076          B4   19920618
     RO 90952             B3   19870227      RO 1985-118055        19850319 <--
     CS 249539            B2   19870312      CS 1985-1920          19850319 <--
     CN 85101028          A    19870117      CN 1985-101028        19850401 <--
     CN 1008733           B    19900711
     CN 85101795              A       19870408    CN 1985-101795          19850401 <--
     CN 1003855               B       19890412
     FI 8904540               A       19890926    FI 1989-4540            19890926 <--
     FI 82449                 B       19901130
     FI 82449                 C       19910311
     JP 04235165              A2      19920824    JP 1991-132826          19910604 <--
     JP 05061269              B4      19930906
RIORITY APPLN. INFO.:                             US 1984-590659       A2 19840319
                                                  US 1984-684634       A  19841221
                                                  EP 1985-301808       A  19850315
                                                  FI 1985-1069         A  19850318
                                                  IL 1985-74631        A  19850318
THER SOURCE(S):          CASREACT 105:24187
I
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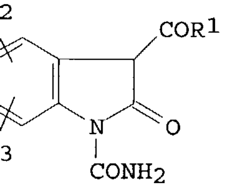


I

B   Oxindoles I [R1 = C1-6 alkyl, C3-7 cycloalkyl, (un)substituted Ph, naphthyl, (CH2)nQR (Q = divalent heterocycle radical; R = H, C1-3 alkyl), etc.; R2 = H, F, Br, Cl, C1-4 alkyl, C3-7 cycloalkyl, C1-4 alkoxy, alkylthio, -sulfinyl, -sulfonyl, NO2, Ph, C2-4 alkanoyl, Bz, thenoyl, C2-4 alkanamido, BzNH, di-C1-3 alkylsulfamoyl, CF3; R3 = H, F, Cl, Br, C1-4 alkyl, C3-7 cycloalkyl, C1-4 alkoxy, alkylthio, CF3; R2R3 = 4,5-, 5,6-, 6,7-OCH2O or OCH2CH2O, (CH2)n (n = 3,4), CH:CHCH:CH, XCH2CH2 (X = O, S), XCH:CH], useful as analgesics and antiinflammatories at 0.01-1.0 g/day, were prepared 5-Chloro-2-oxindole reacted with Me2CHCONCO in refluxing PhMe to give N-isobutyryl-5-chloro-2-oxindole-1-carboxamide which was hydrolyzed with 1N KOH to give 5,2-Cl(H2NCONH)C6H3CH2CO2H. This was cyclized with (F3CCO)2O in refluxing F3CCO2H 1 h to give 5-chloro-2-oxindole-1-carboxamide which was acylated with 2-thenoyl chloride in DMF and 4-(dimethylamino)pyridine to give I (R1 = 2-thienyl, R2 = 5-Cl, R3 = H).

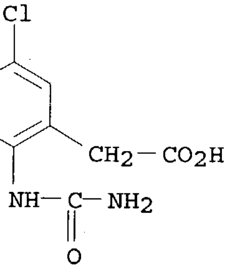
T   **100666-71-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of)

N   100666-71-5 CAPLUS

N   Benzeneacetic acid, 2-[(aminocarbonyl)amino]-5-chloro- (9CI) (CA INDEX NAME)



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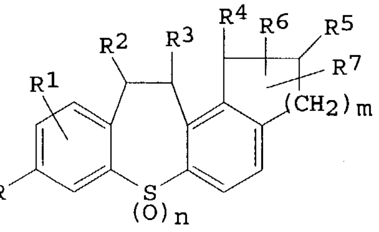
9   ANSWER 9 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
CCESSION NUMBER:         1986:68766  CAPLUS
OCUMENT NUMBER:          104:68766
 TLE:                    6H-Dibenzo[b,f]thiepin compounds
NVENTOR(S):              Williams, Haydn; Rokach, Joshua
ATENT ASSIGNEE(S):       Merck Frosst Canada, Inc., Can.
```

SOURCE: Eur. Pat. Appl., 55 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 138533	A2	19850424	EP 1984-306816	19841005 <--
EP 138533	A3	19860122		
EP 138533	B1	19890412		
R: CH, DE, FR, GB, IT, LI, NL				
US 4622403	A	19861111	US 1983-540480	19831011 <--
CA 1245220	A1	19881122	CA 1984-465055	19841010 <--
JP 60097976	A2	19850531	JP 1984-211560	19841011 <--

PRIORITY APPLN. INFO.: US 1983-540480 A 19831011
OTHER SOURCE(S): CASREACT 104:68766
GI



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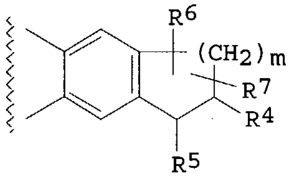

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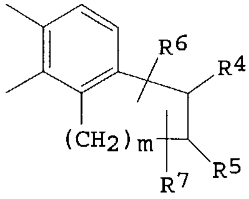

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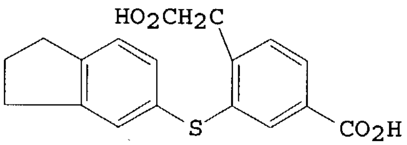
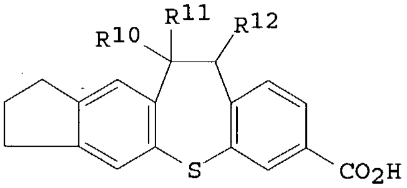


IV



V

AB Dibenzo[b,f]thiepins I-III [R = 5-tetrazolyl, 5-tetrazolylmethyl, 3-hydroxy-1,2,5-thiadiazol-4-yl, 4-hydroxy-2,5-dioxo-Δ3-pyrrolin-3-yl, (CH2)xCOR8, (un)masked CHO, (CH2)yOR9; R1, R6, R7 = H, halogen, NO2, alkyl, (di)(alkyl)amino, alkanoyl, OH, alkoxy, acyloxy, alkylthio, CF3S, CF3, alkylsulfinyl, alkylsulfonyl; R6R7 = O; R2-R5 = H; R2R3, R4R5 = bond; R8 = OH, 2-imino-3-methylthiazolidine, (5-methyl-2-oxo-1,3-dioxolen-4-yl)methoxy, (un)substituted alkoxy, NH2; R9 = H, alkylcarboxy, alkylcarboxamido, acyloxyalkyl, (un)substituted acyl; n = 0-2; m = 1, 2; x, y = 0-4] were prepared Thus, 5-indanthiol and 4-carboxy-2-iodophenylacetic acid were refluxed with powdered Cu-KOH aqueous to give diacid IV, which was cyclized by CF3CO2H-(CF3CO)2O to give benzindenothiepin V (R10R11 = O, R12 = H). Reduction of the latter compound with NaBH4 gave V (R10 = OH, R11 = R12 = H), which was dehydrated by H2SO4-AcOH to give V (R10R12 = bond, R11 = H). I are antagonists and biosynthesis inhibitors of contractile prostaglandins (no data).

T **83209-41-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(arylation by, of mercaptoindan)

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RN   83209-41-0  CAPLUS
CN   Benzeneacetic acid, 4-carboxy-2-iodo- (9CI)  (CA INDEX NAME)
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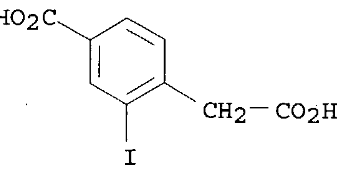

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L9   ANSWER 10 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        1984:591291  CAPLUS
DOCUMENT NUMBER:         101:191291
TITLE:                   Synthesis of biological markers in fossil fuels.  2.
                         Synthesis and carbon-13 NMR studies of substituted
                         indans and tetralins
AUTHOR(S):               Adamczyk, Maciej; Watt, David S.; Netzel, Daniel A.
CORPORATE SOURCE:        Dep. Chem., Univ. Wyoming, Laramie, WY, 82071, USA
SOURCE:                  Journal of Organic Chemistry (1984), 49(22),
                         4226-37
                         CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 101:191291
AB   Unambiguous syntheses of all possible Me, Et, Pr, and Bu derivs. of indan
     and Tetralin were developed using the Kumada coupling procedure involving
     the reaction of aryl or vinyl halides with Grignard reagents in the
     presence of [1,3-bis(diphenylphosphino)propyl]nickel(II) chloride.  An
     anal. of the 13C NMR spectra of these compds. was also completed.
IT   18698-97-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reduction of)
RN   18698-97-0  CAPLUS
CN   Benzeneacetic acid, 2-bromo- (9CI)  (CA INDEX NAME)
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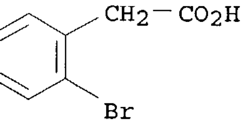

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L9   ANSWER 11 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        1983:505277  CAPLUS
DOCUMENT NUMBER:         99:105277
TITLE:                   Carboxylic acid derivatives and drugs containing them
INVENTOR(S):             Witte, Ernst Christian; Wolff, Hans Peter; Hagenbruch,
                         Bernd; Stegmeier, Karlheinz; Pill, Johannes
PATENT ASSIGNEE(S):      Boehringer Mannheim G.m.b.H. , Fed. Rep. Ger.
SOURCE:                  Ger. Offen., 97 pp.
                         CODEN: GWXXBX
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND  DATE          APPLICATION NO.        DATE
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     DE 3139970           A1   19830428      DE 1981-3139970        19811008 <--
     AU 530448            B2   19830714      AU 1982-88898          19820930 <--
     AU 8288898           A1   19830414
     EP 76996             A1   19830420      EP 1982-109134         19821004 <--
     EP 76996             B1   19860102
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         R:  AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE
     AT 17242              E      19860115    AT 1982-109134        19821004 <--
     JP 58072575           A2     19830430    JP 1982-174072        19821005 <--
     ZA 8207284            A      19830928    ZA 1982-7284          19821005 <--
     DD 204093             A5     19831116    DD 1982-243801        19821005 <--
     DK 8204434            A      19830409    DK 1982-4434          19821006 <--
     HU 27707              O      19831028    HU 1982-3205          19821006 <--
     FI 8203409            A      19830409    FI 1982-3409          19821007 <--
     ES 516311             A1     19830616    ES 1982-516311        19821007 <--
     US 4616086            A      19861007    US 1984-657032        19841001 <--
PRIORITY APPLN. INFO.:                        DE 1981-3139970       19811008
                                              US 1982-422638        19820924
                                              EP 1982-109134        19821004
OTHER SOURCE(S):         CASREACT 99:105277
GI
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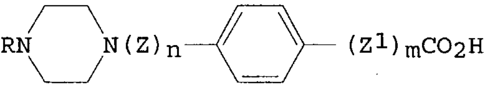

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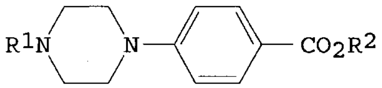

II

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AB   Piperazines I [R = H, (un)substituted alkyl, aryl, acyl; Z = alkylene; Z1
     = alkylene, alkenylene; n, m = 0, 1] were prepared  Thus, 4-H2NC6H4CO2Et was
     cyclocondensed with (ClCH2CH2)2NH to give 55% II (R1 = H, R2 = Et).  This
     was alkylated with Me(CH2)5Br to give 59% II [R1 = Me(CH2)5, R2 = Et],
     which was saponified to give 78% II [R1 = Me(CH2)5, R2 = H].  I are
     hypolipemics (no data).
IT   1878-66-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (acylation by, of piperazines)
RN   1878-66-6  CAPLUS
CN   Benzeneacetic acid, 4-chloro- (9CI)  (CA INDEX NAME)
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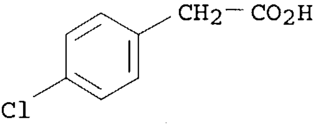

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L9   ANSWER 12 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        1983:89316  CAPLUS
DOCUMENT NUMBER:         98:89316
TITLE:                   Transalkylation and transphenylation of quaternary
                         pyridinium salts:  conversion of primary amines into
                         bis-homologous acids
AUTHOR(S):               Elshafie, Sayed Mahmoud M.
CORPORATE SOURCE:        Fac. Sci., Minia Univ., Minia, Egypt
SOURCE:                  Chimia (1982), 36(9), 343-5
                         CODEN: CHIMAD; ISSN: 0009-4293
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 98:89316
GI
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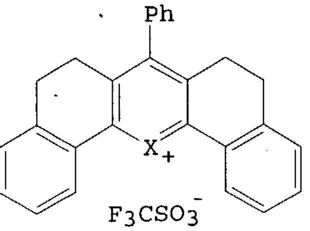
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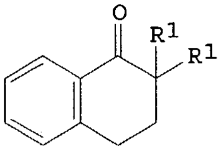
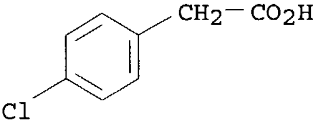

IV

AB RNH2 [I, R = alkyl, (un)substituted Ph] were converted to RCH2CO2H (II) in three steps. I were treated with III (X = O) to give III (X = NR), which were treated with the Na salt of R1CH2CO2Et (R1 = cyano, CO2Et) to give RR1CHCO2Et. Hydrolysis-**decarboxylation** of the latter gave II.

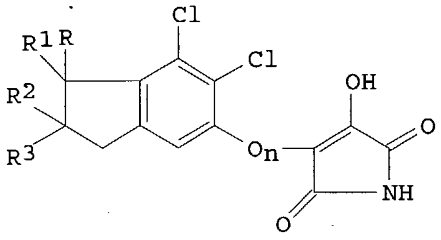
IT **1878-66-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from chloroaniline)
RN 1878-66-6 CAPLUS
CN Benzeneacetic acid, 4-chloro- (9CI) (CA INDEX NAME)



L9 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:527490 CAPLUS
DOCUMENT NUMBER: 97:127490
TITLE: 4-Substituted-3-hydroxy-3-pyrroline-2,5-dione inhibitors of glycolic acid oxidase
INVENTOR(S): Cragoe, Edward J., Jr.; Rooney, Clarence S.; Williams, Haydn W. R.
PATENT ASSIGNEE(S): Merck and Co., Inc. , USA
SOURCE: S. African, 30 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
ZA 8006787	A	19811028	ZA 1980-6787		19801104	<--
US 4342776	A	19820803	US 1979-91294		19791105	<--
PRIORITY APPLN. INFO.:			US 1979-91294	A	19791105	

OTHER SOURCE(S): CASREACT 97:127490
GI



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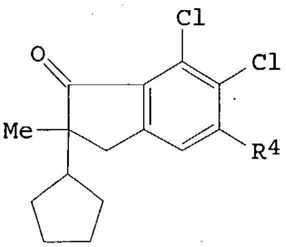
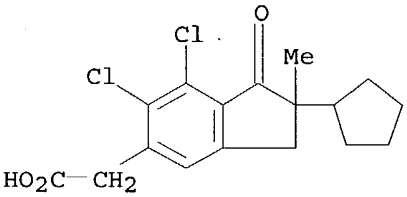


II, R^4=OH

III, R^4=CH_2CONH_2

AB The title compds. I (R = H, R1 = OH; RR1 = O; R2 = C1-3 alkyl; R3 = C1-3 alkyl, C4-6 cycloalkyl; n = 0, 1), useful as glycolate oxidase inhibitors and thus useful in treating and preventing Ca oxalate kidney and bladder stone formation (no data), were prepared Thus, I (RR1 = O, R2 = Me, R3 = cyclopentyl, n = 0) was prepared in 6 steps from indanone II and F3CSO2Cl via acetamide III.

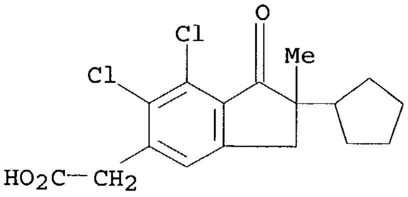
IT **71500-84-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 71500-84-0 CAPLUS
CN 1H-Indene-5-acetic acid, 6,7-dichloro-2-cyclopentyl-2,3-dihydro-2-methyl-1-oxo- (9CI) (CA INDEX NAME)



IT **71500-85-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 71500-85-1 CAPLUS
CN 1H-Indene-5-acetic acid, 6,7-dichloro-2-cyclopentyl-2,3-dihydro-2-methyl-1-oxo-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

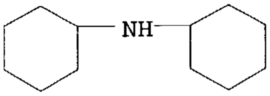
CM 1

CRN 71500-84-0
CMF C17 H18 Cl2 O3



CM 2

CRN 101-83-7
CMF C12 H23 N



L9 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:406906 CAPLUS
DOCUMENT NUMBER: 95:6906
TITLE: Indanacetic acid compounds
INVENTOR(S): Cragoe, Edward J., Jr.; Williams, Haydn W. R.; Woltersdorf, Otto W., Jr.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4249021	A	19810203	US 1979-15095	19790226 <--
PRIORITY APPLN. INFO.:			US 1979-15095	19790226

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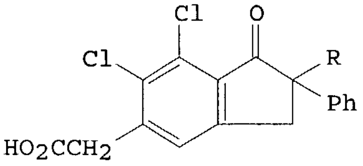

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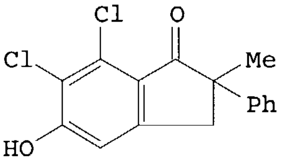
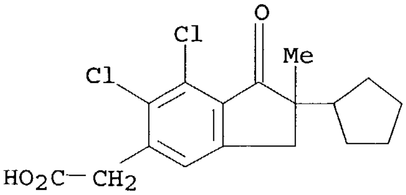


II

AB The title compds. I (R = alkyl), useful as diuretics (no data), are prepared Thus, II was converted to the methanesulfonate, which reacted with $CH_2(CO_2Et)_2$ followed by hydrolysis and **decarboxylation** to give I (R = Me).

IT **71500-84-0P 71500-85-1P 71500-88-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of diuretic)

RN 71500-84-0 CAPLUS
CN 1H-Indene-5-acetic acid, 6,7-dichloro-2-cyclopentyl-2,3-dihydro-2-methyl-1-oxo- (9CI) (CA INDEX NAME)



RN 71500-85-1 CAPLUS
CN 1H-Indene-5-acetic acid, 6,7-dichloro-2-cyclopentyl-2,3-dihydro-2-methyl-1-oxo-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

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     CRN  71500-84-0
     CMF  C17 H18 Cl2 O3
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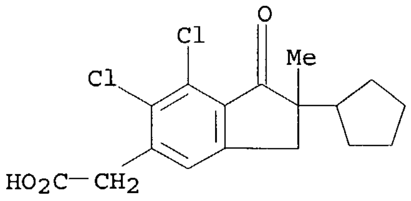

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     CRN  101-83-7
     CMF  C12 H23 N
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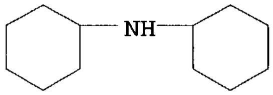

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RN   71500-88-4  CAPLUS
CN   1H-Indene-5-acetic acid, 6,7-dichloro-2,3-dihydro-2-methyl-1-oxo-2-phenyl-
     (9CI)  (CA INDEX NAME)
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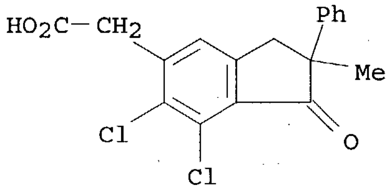

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L9   ANSWER 15 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1981:156942  CAPLUS
DOCUMENT NUMBER:          94:156942
TITLE:                    Substituted 6-phenyl-5,6,7,8-tetrahydro-1,2,4-triazolo-
                          [4,3-a]pyridines
INVENTOR(S):              Trust, Ronald I.; Albright, Jay D.
PATENT ASSIGNEE(S):       American Cyanamid Co., USA
SOURCE:                   U.S., 12 pp.
                          CODEN: USXXAM
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
     ---------------      ----   --------    --------------------   --------
     US 4244953            A     19810113    US 1979-87907          19791024 <--
PRIORITY APPLN. INFO.:                       US 1979-87907          19791024
GI
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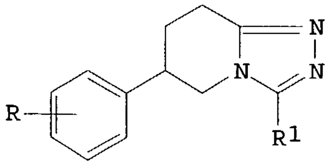

I

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AB    2-Hydrazinopyridines reacted with ortho esters to give triazolopyridines
      which were hydrogenated to yield title compds. I (R = H, alkyl, F, Cl, Br,
      CF3, cyano, CO2H, alkoxycarbonyl, carbamoyl, NH2, NHAc, dialkylamino,
      alkoxy; R1 = H, alkyl), useful as anxiolytic agents (no data).
      2-Chloro-5-phenylpyridine was heated with N2H4 and pyridine to give the
      2-hydrazino analog, the latter and MeC(OEt)3 was refluxed, and the product
      was hydrogenated over Pd/C to give I (R = H, R1 = Me).
IT    331-25-9
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (condensation reaction of, with DMF, decarboxylation in)
RN    331-25-9  CAPLUS
CN    Benzeneacetic acid, 3-fluoro- (9CI)  (CA INDEX NAME)
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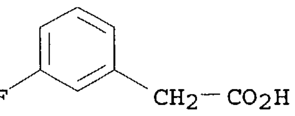

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L9   ANSWER 16 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1981:139815  CAPLUS
DOCUMENT NUMBER:          94:139815
TITLE:                    Substituted 3-alkyl-6-phenyl-1,2,4-triazolo[4,3-
                          a]pyridines and pharmaceutical compositions containing
                          them
INVENTOR(S):              Trust, Ronald Irving; Albright, Jay Donald
PATENT ASSIGNEE(S):       American Cyanamid Co., USA
SOURCE:                   Eur. Pat. Appl., 38 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE       APPLICATION NO.        DATE
     ---------------     ----   --------   --------------------   --------
     EP 17438             A1    19801015   EP 1980-300971         19800328 <--
     EP 17438             B1    19830302
         R:  AT, BE, CH, DE, FR, GB, IT, LU, NL, SE
     US 4242515           A     19801230   US 1979-24849          19790328 <--
     CA 1146554           A1    19830517   CA 1980-344556         19800129 <--
     AU 8055196           A1    19801002   AU 1980-55196          19800204 <--
     AU 533295            B2    19831117
     DD 150466            C     19810902   DD 1980-219909         19800325 <--
     JP 55130977          A2    19801011   JP 1980-38313          19800327 <--
     HU 24142             O     19821228   HU 1980-722            19800327 <--
     HU 181695            B     19831128
     AT 2674              E     19830315   AT 1980-300971         19800328 <--
PRIORITY APPLN. INFO.:                     US 1979-24849       A  19790328
                                           EP 1980-300971      A  19800328
GI
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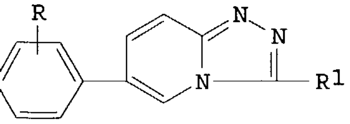
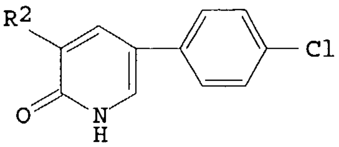


I



II

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AB    Anxiolytic (no data) triazolopyridines I (R = H, alkyl, alkoxy, F, Cl, Br,
      CF3, cyano, CO2H, alkoxycarbonyl, CONH2, NO2, NH2, acylamino, alkylamino,
      dialkylamino; R1 = alkyl) were prepared  Thus 4-ClC6H4CH2CO2H was subjected
      to Vilsmeyer reaction and 4-ClC6H4C(:CHNMe2)CHO treated with NCCH2CONH2 to
      give II (R2 = cyano), which was hydrolyzed to the acid and
```
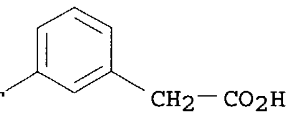

decarboxylated to II (R2 = H). Chlorination of II (R2 = H) gave 2-chloro-5-(4-chlorophenyl)pyridine, which was treated with N2H4 and cyclized with MeC(OEt)3 to give I (R = 4-Cl, R1 = Me).

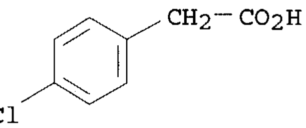
T **331-25-9 1878-66-6 2444-36-2**

RL: RCT (Reactant); RACT (Reactant or reagent)
(Vilsmeyer reaction of)

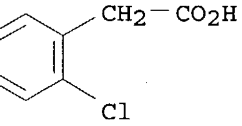
N 331-25-9 CAPLUS
N Benzeneacetic acid, 3-fluoro- (9CI) (CA INDEX NAME)



N 1878-66-6 CAPLUS
N Benzeneacetic acid, 4-chloro- (9CI) (CA INDEX NAME)



N 2444-36-2 CAPLUS
N Benzeneacetic acid, 2-chloro- (9CI) (CA INDEX NAME)

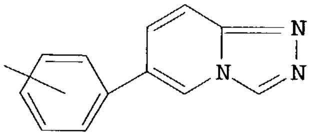


9 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN

CCESSION NUMBER: 1981:30760 CAPLUS
OCUMENT NUMBER: 94:30760
ITLE: Substituted 6-phenyl-1,2,4-triazolo[4,3-a]pyridines
NVENTOR(S): Albright, Jay D.; Trust, Ronald I.
ATENT ASSIGNEE(S): American Cyanamid Co., USA
OURCE: U.S., 11 pp.
CODEN: USXXAM
OCUMENT TYPE: Patent
ANGUAGE: English
AMILY ACC. NUM. COUNT: 1
ATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4209626	A	19800624	US 1979-20886	19790315 <--
RIORITY APPLN. INFO.:			US 1979-20886	19790315

I

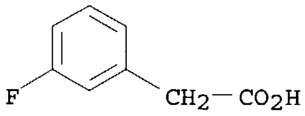


I

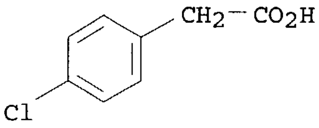
AB Triazolopyridines I (R = H, C1-4 alkyl, C1-4 alkoxy, F, Cl, Br, CF3, cyano, CO2H, C2-5 alkoxycarbonyl, CONH2, NO2, NH2, AcNH, C1-4 alkylamino, dialkylamino), useful as antihypertensives (no data), were prepared Thus, 4-ClC6H4C(CHO):CHNMe2, prepared by the condensation of DMF and 4-ClC6H4CH2CO2H in the presence of POCl3, was cyclocondensed with NCCH2CONH2, hydrolyzed, **decarboxylated**, chlorinated by POCl3, and hydrazinolyzed to give 5-(4-chlorophenyl)-2-hydrazinopyridine (II). The cyclocondensation of II and HC(OEt)3 gave I (R = 4-Cl).

IT **331-25-9 1878-66-6 2444-36-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with DMF)

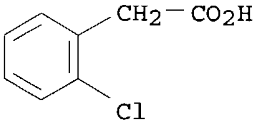
RN 331-25-9 CAPLUS
CN Benzeneacetic acid, 3-fluoro- (9CI) (CA INDEX NAME)



RN 1878-66-6 CAPLUS
CN Benzeneacetic acid, 4-chloro- (9CI) (CA INDEX NAME)

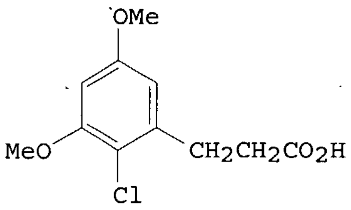


RN 2444-36-2 CAPLUS
CN Benzeneacetic acid, 2-chloro- (9CI) (CA INDEX NAME)

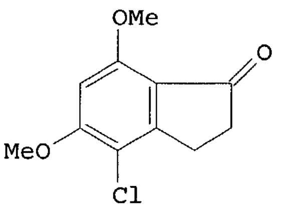


L9 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN

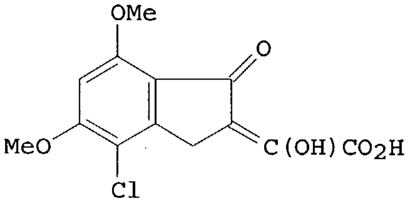
ACCESSION NUMBER: 1980:567820 CAPLUS
DOCUMENT NUMBER: 93:167820
TITLE: Synthesis of 6-chloro-3,5-dimethoxyhomophthalic acid, a key intermediate for the synthesis of radicicol and natural isocoumarin
AUTHOR(S): Nozawa, Koohei; Nakajima, Shoichi; Kawai, Kenichi
CORPORATE SOURCE: Hoshi Coll. Pharm., Tokyo, 142, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (**1980**), 28(4), 1112-16
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



II



III



IV

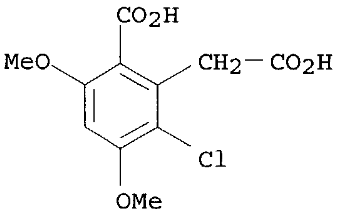
AB 6-Chloro-3,5-dimethoxyhomophthalic acid (I) was prepared via a sequence of reactions including cyclization of propionic acid II to III and oxidative decomposition of IV to I as key steps.

IT **75177-70-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for synthesis of radicicol and natural isocoumarin)

RN 75177-70-7 CAPLUS

CN Benzeneacetic acid, 2-carboxy-6-chloro-3,5-dimethoxy- (9CI) (CA INDEX NAME)



L9 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:514154 CAPLUS
DOCUMENT NUMBER: 93:114154
TITLE: Amino-substituted phenyl and heteroaryl compounds and pharmaceutical compositions containing them
INVENTOR(S): Shepherd, Robert Gordon
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: Eur. Pat. Appl., 492 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 3663	A2	19790822	EP 1979-300167	19790202 <--
EP 3663	A3	19801112		
R: BE, CH, DE, FR, GB, IT, NL, SE				
US 4243609	A	19810106	US 1978-874433	19780202 <--
US 4227014	A	19801007	US 1978-881457	19780227 <--
US 4245097	A	19810113	US 1978-881456	19780227 <--
US 4230878	A	19801028	US 1978-884673	19780308 <--
US 4205085	A	19800527	US 1978-884941	19780309 <--
US 4211783	A	19800708	US 1978-890569	19780320 <--
US 4230628	A	19801028	US 1978-895574	19780412 <--
ZA 7900464	A	19801029	ZA 1979-464	19790119 <--

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     ES 477314             A1     19800301    ES 1979-477314        19790131 <--
     US 4281018            A      19810728    US 1980-150511        19800516 <--
     US 4311846            A      19820119    US 1980-176890        19800811 <--
     US 4333940            A      19820608    US 1980-176958        19800811 <--
     US 4423051            A      19831227    US 1981-285206        19810720 <--
     US 4411903            A      19831025    US 1981-313853        19811022 <--
PRIORITY APPLN. INFO.:                        US 1978-874433        19780202
                                              US 1978-881456        19780227
                                              US 1978-881457        19780227
                                              US 1978-884673        19780308
                                              US 1978-884941        19780309
                                              US 1978-888268        19780320
                                              US 1978-890569        19780320
                                              US 1978-895574        19780412
                                              US 1980-137199     A3 19800404
                                              US 1980-176890     A3 19800811
OTHER SOURCE(S):         CASREACT 93:114154
AB   A wide variety of title compds. (.apprx.700 compds.) were prepared by
     numerous methods as hypolipidemics (no data).  Thus, heating
     cyclohexylmethyl bromide with 4-H2NC6H4CO2Et in P(O)(NMe2)3 20 h gave an
     ester whose saponification gave 4-[(cyclohexylmethyl)amino]benzoic acid.
IT   73781-65-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN   73781-65-4  CAPLUS
CN   Benzeneacetic acid, 2-fluoro-4-(hexadecylamino)- (9CI)  (CA INDEX NAME)
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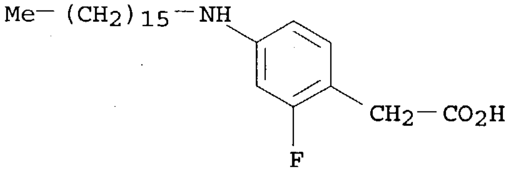

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L9   ANSWER 20 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        1980:128644  CAPLUS
DOCUMENT NUMBER:         92:128644
TITLE:                   Nucleophilic displacement of activated aryl triflates.
                         A new synthesis of oxindoles and arylacetic acids
AUTHOR(S):               Atkinson, Joseph G.; Wasson, Burton K.; Fuentes, Jose
                         J.; Girard, Yves; Rooney, C. Stanley; Engelhardt,
                         Edward L.
CORPORATE SOURCE:        Merck Frosst Lab., Pointe Claire/Dorval, QC, H9R 4P8,
                         Can.
SOURCE:                  Tetrahedron Letters (1979), (31), 2857-60
                         CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 92:128644
AB   2-Nitroaryl triflates underwent base-catalyzed nucleophilic displacement
     by (MeO2C)2C-H giving di-Me nitroarylmalonates, which were converted to
     nitroarylacetic acids and oxindoles.  E.g., 4,2-Me(HO)C6H3NO2 was treated
     sequentially with CF3SO2Cl/Et3N in Me2CO, CH2(CO2Me)2/NaH in DMF
     (20°, 20 h) and, HCl/HOAc (reflux 18 h) to give 95%
     5,2-Me(O2N)C6H3CH2CO2H which on hydrogenation in MeOH over Pd, gave 88%
     5-methyloxindole.  The triflate displacement also constitutes a new,
     practical preparation of nitroarylacetic acids.
IT   66949-40-4P 73088-11-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN   66949-40-4  CAPLUS
CN   Benzeneacetic acid, 2-bromo-4-nitro- (9CI)  (CA INDEX NAME)
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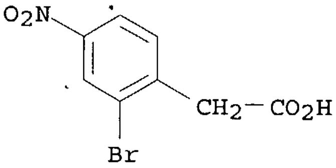
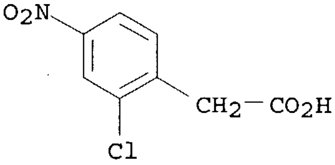


RN 73088-11-6 CAPLUS
CN Benzeneacetic acid, 2-chloro-4-nitro- (9CI) (CA INDEX NAME)



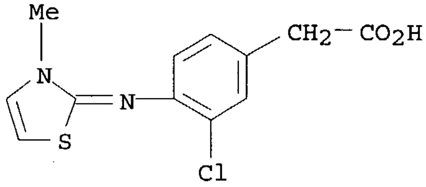
L9 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:16658 CAPLUS
DOCUMENT NUMBER: 86:16658
TITLE: Thiazoline derivatives and their salts
INVENTOR(S): Maeda, Ryozo; Hirose, Katsumi
PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2554863	A1	19760616	DE 1975-2554863	19751205 <--
DE 2554863	C2	19840823		
JP 51075065	A2	19760629	JP 1974-140776	19741206 <--
CA 1060024	A1	19790807	CA 1975-240770	19751127 <--
GB 1476594	A	19770616	GB 1975-49094	19751128 <--
SE 7513574	A	19760608	SE 1975-13574	19751202 <--
SE 430064	B	19831017		
SE 430064	C	19840126		
DK 7505512	A	19760607	DK 1975-5512	19751205 <--
DK 144473	B	19820315		
DK 144473	C	19820830		
FR 2293200	A1	19760702	FR 1975-37369	19751205 <--
CH 621783	A	19810227	CH 1975-15879	19751205 <--
NL 7514284	A	19760609	NL 1975-14284	19751208 <--
CH 624109	A	19810715	CH 1980-6772	19800909 <--
PRIORITY APPLN. INFO.:			JP 1974-140776	19741206
			CH 1975-15879	19751205

GI For diagram(s), see printed CA Issue.

AB Thiazolines I (R1 = H, Me; R2 = H, 2-, 3-, 4-Cl, 2-, 3-, 4-F, 2-, 3-Me, 2-, 3-CF3; R3 = H; R4 = H, Me; allyl; R5 = H, Me; CHR1CO2R group at 3, 4, 4', or 5'; R1 = R4 = Me, R2 = 2-Cl, R3 = 6-Cl, R5 = H, Me; R1 = R4 = R5 = Me, R2 = 3-Me, R3 = 2-Cl, CHR1CO2R group at 4) and (or) their Ca salts (30 compds.), useful as analgesics, inflammation inhibitors, and antipyretics, were prepared Thus, thiazole II (R1 = Me, R2 = R3 = R5 = R6 = H, CR1R6CO2Et at 4) (III) was quaternized with MeI in EtOH 20 hr at 50-5° to give 84% III 3'-methiodide which was dehydrohalogenated to give 83% IV (R1 = R4 = Me, R2 = R3 = R5 = H, CHR1CO2R at 4). This was saponified to give 73% the corresponding I. I (R1 = Me, R2 = 3-Cl, R3 = R5 = H, R6 = CO2Et, CR1R6CO2Et at 4) was similarly quaternized, the quaternary salt dehydrohalogenated to 94.5% **malonate**, and the ester saponified and **decarboxylated** to give I (R1 = R4 = Me, R2 = 3-Cl, R3 = R5 = H, CHR1CO2R at 4). I (R1 = R4 = Me, R2 = 2-F, R3 = R5 = H, CHR1CO2R at 4), e.g., had ED50 11 (method of Bliss, AcOH writhing test), 0.25 (Bliss,

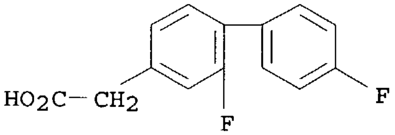
carrageenin edema), and 1.3 (Bliss, antipyretic activity).
IT **61225-47-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61225-47-6 CAPLUS
CN Benzeneacetic acid, 3-chloro-4-[(3-methyl-2(3H)-thiazolylidene)amino]- (9CI) (CA INDEX NAME)



L9 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:520230 CAPLUS
DOCUMENT NUMBER: 81:120230
TITLE: Analgesic, antiinflammatory, and antipyretic 2-biphenylylpropionic acid derivatives
INVENTOR(S): Adams, Stewert Sanders; Armitage, Bernard J.; Nicholson, John S.
PATENT ASSIGNEE(S): Boots Co. Ltd.
SOURCE: Brit., 9 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1359987	A	19740717	GB 1970-48405	19710917 <--
PRIORITY APPLN. INFO.:			GB 1970-48405	19710917

GI For diagram(s), see printed CA Issue.
AB Eight title compds. I (R = F, Br; R1 = H, R2 = F, Br, or R1 = F, Br, R2 = H) and some esters and salts of I were prepared Thus, I (R = R1 = F, R2 = H) was prepared by **decarboxylation** of Et 2-(2', 4'-difluoro-4-biphenylyl)-2-methylmalonate. The **malonate** was prepared in 3 stages from 2,4-difluorobiphenyl which was obtained by a modified Gomberg reaction of 2,4-F2C6H3NH2 and BuNO2 in C6H6. I-containing compns. for capsules and tablets were described. I have long lasting antiinflammatory, analgesic, and antipyretic effects.
IT **53591-85-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 53591-85-8 CAPLUS
CN [1,1'-Biphenyl]-4-acetic acid, 2,4'-difluoro- (9CI) (CA INDEX NAME)



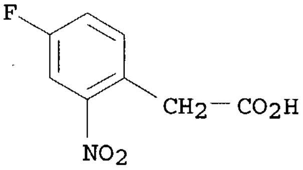
L9 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:58051 CAPLUS
DOCUMENT NUMBER: 78:58051
TITLE: 4-Fluoro-2-nitrophenylacetone
INVENTOR(S): Sasajima, Kikuo; Nakao, Masaru; Maruyama, Isamu; Katayama, Shigenari; Yamamoto, Hisao

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
JP 47038947	B4	19721216	JP 1971-25539	19710419	<--

AB Et (4-fluoro-2-nitrophenyl)pyruvate (K salt) in an aqueous solution of KOH was stirred with 30% H_2O_2, the resulting (4-fluoro-2-nitrophenyl)acetic acid treated with $SOCl_2$, the resulting acid chloride treated with di-Et ethoxymagnesiummalonate, and the resulting di-Et (4-fluoro-2-nitrophenyl)acetylmalonate subjected to an acid hydrolysis and **decarboxylation** to give the title compound, useful as a central nerve depressant and antiinflammatory drug.

IT **39616-95-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionyl chloride)
RN 39616-95-0 CAPLUS
CN Benzeneacetic acid, 4-fluoro-2-nitro- (9CI) (CA INDEX NAME)



L9 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:96611 CAPLUS
DOCUMENT NUMBER: 70:96611
TITLE: 4-(1-Pyrryl)phenylacetic acid and derivatives
INVENTOR(S): Denss, Rolf; Clauson-Kaas, Niels; Ostermayer, Franz
PATENT ASSIGNEE(S): Geigy, J. R., A.-G.
SOURCE: S. African, 75 pp.
CODEN: SFXXAB
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PATENT INFORMATION:

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ZA 6706465		19680604			<--
CH 480333			CH		
CH 480334			CH		
CH 485708			CH		
CH 485709			CH		
CH 485710			CH		
CH 485711			CH		
CH 485712			CH		
CH 485713			CH		
CH 485714			CH		
CH 485715			CH		
CH 499515			CH		
CH 500973			CH		
CH 542843			CH		
DE 1695044			DE		
ES 346585			ES		
FR 1543100			FR		
FR 7236			FR		
FR 7237			FR		
GB 1200204			GB		

US 3579535	19710000	US	<--
US 3665010	19720000	US	<--
US 3665011	19720000	US	<--
US 3673212	19720000	US	<--
US 3689656	19720000	US	<--

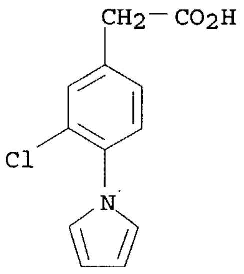
PRIORITY APPLN. INFO.:	CH	19661031
	CH	19670807

AB A series of title compds. is prepared Thus, 179 g. 2-(4-aminophenyl)butanoic acid (I) and 132 g. 2,5-di-methoxytetrahydrofuran (II) in 200 ml. HOAc refluxed 30 min. and fractionally distilled, gave 2-[4-(1-pyrryl)phenyl]butanoic acid (Ia), b0.5 180-200°, m. 112-13°, (1:1 C6H6-cyclohexane); Me ester m. 56-8° (MeOH); Et ester b0.1 118-23°, n2D5 1.5502, m. 29-31°; amide m. 145-6° (Et2O), Me2NCH2CH2OH salt, m. 96-100° (C6H6), K salt m. 255° (10:1 dioxane-iso-PrOH). Similarly prepared were p-(1-pyrryl)hydratropic acid, m. 166-8°, and 2-[4-(1-pyrryl)phenyl]pentanoic acid, m. 108-9°. 3-Methylfuran was converted into 2,5-dimethoxy-3-methyl-2,5-dihydrofuran, b. 171-2°, n2D5 1.4358, which was reduced to 2,5-dimethoxy-3-methyltetrahydrofuran, b. 157-8°, n2D5 1.4169. 2,4-dimethoxy-3-methyltetrahydrofuran and I gave 2-[4-(3-methyl-1-pyrryl)-phenyl]butanoic acid, m. 138-9°. A mixture of 30.2 g. p-H2NC6H4CH2CO2H and 26.4 g. II in 40 ml. HOAc was refluxed 30 min. and worked up to give p-(1-pyrryl)phenylacetic acid (III), m. 180-2° (C6H6); Me ester b0.1 120-6°, b0.3 126-38°, b1.5 148-50°, n2D5 1.5770, m. 43-4° (CCl4-ligroine); Et ester b0.2 129-31°, n2D5 1.5529, m. 55-6°; Bu ester m. 40-1° (iso-PrOH-C6H6); Et3N salt m. 67-73°. A mixture of 3.58 g. I and 2.28 g. (AcCH2)2 in 7 ml. HOAc was refluxed 30 min. and worked up to give 2-[4-(2,5-dimethyl-1-pyrryl)phenyl]butanoic acid, m. 154-5°. Action of NaNH2 from 1.45 g. Na in 150 ml. liquid NH3 on 5.03 g. III, followed by addition of 2.73 g. EtBr in 5 ml. Et2O and refluxing 30 min. gave Ia. From III. NaNH2, and R1X (X = Br or I) were likewise prepared α-R1-substituted derivs. of Ia (R1 and m.p. given): Pr, 108-9°; iso-Pr, 148-9°; allyl, 102-5°; propargyl, 122-3°; and Bu, 96-8° (methylcyclohexane). II (13.2 g.) and 13.5 g. 4-H2NC6H4Ac in 25 ml. HOAc, refluxed 2.5 hrs., gave 4-(1-pyrryl)acetophenone (IV), m. 120-2° (iso-PrOH). Also prepared were 3-bromo-4-(1-pyrryl)acetophenone; 3-methyl-4-(1-pyrryl)acetophenone; 3-methoxy-4-(1-pyrryl)-acetophenone, b0.05 220°, m. 58-64°; 2-chloro-4-(1-pyrryl)acetophenone; and Et 4-(1-pyrryl)benzoate (V), b0.01 140-5°, m. 75-6° (MeOH). Saponification of 32 g. V with 12 g. NaOH in 600 ml. EtOH gave 4-(1-pyrryl)benzoic acid (VI), m. 265-70° (decomposition) VI (7.4 g.) was treated with 3.3 ml. SOCl2 and 4.8 g. C5H5N in CH2Cl2 3 hrs. under N, evaporated, the product dispersed in 100 ml. tetrahydrofuran and added to 200 ml. 0.6N CH2N2 in Et2O, and the mixture kept 18 hrs. at room temperature and evaporated to give crude 4-(1-pyrryl)2-diazoacetophenone. Rearrangement of this in 180 ml. MeOH by Ag2O from 2 g. AgNO3 during 4 hrs. gave III. II (17.8 g.), 17.8 g. 4-H2NC6H4CH2CN, and 47 ml. HOAc refluxed 2 hrs. and worked up gave 4-(1-pyrryl)phenylacetonitrile, m. 104-5° (iso-PrOH), which was saponified to III. IV (3.7 g.), 1 g. S, and 4 ml. morpholine refluxed 15 hrs., then mixed with 20 ml. EtOH and 30 ml. 2N NaOH and refluxed 8 hrs., gave 4 g. III. Similarly prepared were: 3-bromo-4-(1-pyrryl)phenylacetic acid; 3-methyl-4-(1-pyrryl)phenylacetic acid, b0.02 190°, n2D2 1.5755; 3-methoxy-4-(1-pyrryl)phenylacetic acid, m. 124-6° (iso-PrOH); and 2-chloro-4-(1-pyrryl)phenylacetic acid. To 2.7 g. Mg and 2.5 ml. absolute EtOH in the presence of a trace of iodine and 0.25 ml. CCl4, diluted with 37.5 ml. Et2O was gradually added 17.6 g. CH2(CO2Et)2 in 10 ml. absolute EtOH and 12.5 ml. absolute Et2O. The mixture was refluxed 3 hrs., cooled, treated with an Et2O solution of 21.5 g. crude 4-nitro-3-methoxybenzoyl chloride, and the mixture refluxed 0.5 hr. and worked up to give 4-nitro-3-methoxyacetophenone (VII), m. 66-8° (Et2O). Reduction of 7.35 g. VII in 90 ml. HOAc at 70° by 30 g. SnCl2 in 30 ml. concentrated HCl, gave 4-amino-3-methoxyacetophenone, m. 66-87° (Et2O-petroleum ether). Addition of 7.5 ml. SOCl2 in 10 ml. C6H6 at 10-20° to 20.7 g. Et 2-(4-aminophenyl)butanoate in 100 ml. C6H6, refluxing 15 min., and distillation gave Et 2-(4-sulfinyliminophenyl)butanoate (VIII), b0.1 125°. Similarly prepared was Et (4-sulfinyliminophenyl)acetate, b0.1 110°. VIII (21.2 g.) and 12 g.

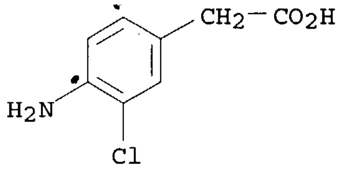
(CH2:CMe)2 in 50 ml. MeCN was refluxed 17 hrs. and the product saponified to give 2-[4-(3,4-dimethyl-1-pyrryl)phenyl]-butanoic acid, m. 131-2° (CCl4). Similarly prepared was 4-(3,4-dimethyl-1-pyrryl)phenylacetic acid, m. 183-5° (MeOH). To a mixture of 80 g. III Et ester and 280 ml. Et2CO3 at 75-80° was added 10 g. Na in 450 ml. EtOH, EtOH distilled until the vapor temperature reached 120°, 200 ml. Et2CO3 added, distillation continued, until the vapor temperature reached 123°, and the mixture worked up to give 88.5 g. di-Et 4-(1-pyrryl)phenylmalonate (IX), m. 80-3° (MeOH). To 2 g. Na in 80 ml. absolute EtOH at 50° was added 24 g. IX in 60 ml. absolute EtOH. After 0.5 hr. at 40-50°, 16 ml. MeI was added. The mixture was refluxed 4 hrs., 16 ml. MeI added, and the mixture refluxed 2 hrs. and worked up to give di-Et methyl[4-(1-pyrryl)phenyl] **malonate** (X), m. 57-8°. Similarly prepared was di-Et ethyl[4-(1-pyrryl)-phenyl]**malonate**, b0.05 215°, n2D3 1.5415. Treatment of 1.9 g. X with 1.4 g. KOH in 5 ml. H2O and 15 ml. BuOH, concentration extraction with Et2O, and acidification gave 2-[4-(1-pyrryl)phenyl]-propionic acid, m. 168-9° (MeOH); Me ester b0.008 123°, n2D5 1.5680, m. 40-1°. To 46.3 g. 4-AcNHC6H4CH2CO2H dispersed in 100 ml. Me2CO and 108 ml. concentrated HCl was added 10.7 g. NaClO3 in 13 ml. H2O at -5° during 1 hr. After 15 min. at 0°, 75 ml. concentrated HCl was added, and the mixture refluxed 2 hrs. and worked up to give 31 g. 4-amino-3-chlorophenylacetic acid, m. 135-7° (iso-PrOH-C6H6). This (27.8 g.) and 19.8 g. II in 40 ml. HOAc gave 54% 3-chloro-4-(1-pyrryl)phenylacetic acid (XI), b0.1 164°, n2D5 1.5976, m. 75-6° (20:1 cyclohexane-C6H6). From XI were prepared 7% 2-[3-chloro-4-(1-pyrryl)-phenyl]butanoic acid, m. 78-80° (cyclohexane) and 2-[3-chloro-4-(1-pyrryl)phenyl]propanoic acid, m. 78-80°. A mixture of 34.6 g. 4-H2NC6H4CHEtCO2H, 38 g. Me 2,5-dimethoxytetrahydrofu-ran-2-carboxylate, and 100 ml. HOAc was refluxed 16 hrs. to give 32.5 g. 1-[4-(1-carboxypropyl)phenyl]-2-pyrrolecarboxylic acid, m. 184-5° (Me2CO), **decarboxylation** of which at 200° gave Ia. Ethylation of 18.2 g. 4-(1-pyrryl)phenylacetonitrile by 10.9 g. EtBr in the presence of NaNH2 gave 2-[4-(1-pyrryl)phenyl]-butryonitrile, m. 38-9°. Ia (4.95 g.) in 30 ml. Me2CO and 8 g. cinchonidine in 25 ml. MeOH were mixed and the solvent was evaporated Recrystn. of the residue from 50 ml. Me2CO gave 11 g. cinchonidine (-)-2-[4-(1-pyrryl)phenyl]butanoate, m. 140° (Me2CO). Acidification of 2 g. of this salt in 50 ml. H2O by 15 ml. 2N HCl precipitated (-)-Ia, m. 130-2° (CCl4), [α]2D5 -39.9°. The mother liquor was evaporated to dryness, the residue suspended in 50 ml. N HCl and extracted with 50 ml. Et2O, and the residue from the extract dissolved in 40 ml. hot iso-PrOH and treated with 1.8 g. (+)-PhCHMeNH2 to give 3.2 g. salt, m. 148-50° (EtOH), [α]2D5 4.40° (MeOH), from 1.25 g. of which was obtained (+)-Ia. I have analgesic, antipyretic, and antiphlogistic activity.

IT **22106-56-5P 22106-57-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 22106-56-5 CAPLUS
CN Acetic acid, (3-chloro-4-pyrrol-1-ylphenyl)- (8CI) (CA INDEX NAME)



RN 22106-57-6 CAPLUS
CN Benzeneacetic acid, 4-amino-3-chloro- (9CI) (CA INDEX NAME)



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L9   ANSWER 25 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1943:33626  CAPLUS
DOCUMENT NUMBER:          37:33626
ORIGINAL REFERENCE NO.:   37:5382d-i
TITLE:                    Iodinated organic compounds as contrast media for
                          radiographic diagnoses. II. Ethyl esters of iodinated
                          straight- and branched-chain phenyl fatty acids
AUTHOR(S):                Plati, J. T.; Strain, W. H.; Warren, S. L.
SOURCE:                   Journal of the American Chemical Society (1943
                          ), 65, 1273-6
                          CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE:            Journal
LANGUAGE:                 Unavailable
AB   cf. C. A. 36, 4491.3.  Ph(CH2)4CO2H (I) can be prepared in 86% yield from Ph
     (CH2)3CH (CO2Et)2 (the latter being obtained in 69% yield); it also
     results in 70% yield from PhCH:CHCHO through the steps PhCH:CHCH:CHAc and
     PhCH:CHCH2CO2H; thus I is a very accessible compound  In the direct
     iodination of Ph(CH2)x CO2H, 1 mol. of the acid in 10 vols. AcOH was
     treated with 1 volume concentrated H2SO4 and 1 equivalent iodine and then with 0.9-1
     part solid NaNO2 in 1 portion; the mixture was heated until the iodine color
     disappeared (20-30 min.); the % yields were: p-IC6H4CH2CO2H 39-45,
     p-IC6H4(CH2)2CO2H (II) 50, p-IC6H4(CH2)3CO2H (III) 27,
     δ-(p-iodophenyl)valeric acid (IV) 50 (m. 109.5-10.5°),
     p-IC6H4(CH2)5CO2H (V) 14, ζ-(p-iodophenyl)heptoic acid (VI) 39 (m.
     93-4.5°).  A mixture of 8.6 g. KIO3, 35.6 g. I, 20.3 g. iodine, 250
     cc. 60% AcOH and 10cc. concentrated H2SO4 refluxed for 3.75 h. (better 10-20
     min.) gives 59% of crude IV.  I (64.1 g.) with 130 cc. concentrated HNO3 (d.
     1.4) and 65 cc. fuming HNO3 (d. 1.5) at 60° for 20 min. gives 28%
     of δ-(p-nitrophenyl)valeric acid, m. 84-5°; reduction with
     Fe(OH)2 in NH4OH gives 42% of the NH2 derivative, m. 113-13.5°; the
     Sandmeyer reaction gives a nearly quant. yield of IV.  Et esters: II, b2
     140°, d2020 1.532, n25D 1.5597; III, b0.8 146-8°, d2020
     1.486, n25D 1.5528; IV, b2 158°, d2020 1.436, n25D 1.5471; V, b2
     158-60°, d2020 1.401, n25D 1.5413; VI, b2.5 175-7°, d2020
     1.367, n25D 1.5367.  CHEt(CO2Et)2 and p-IC6H4CH2Br give 64% of di-Et
     ethyl(p-iodobenzyl)malonate, b2 176-80°, d2020 1.404,
     n25D 1.5348; hydrolysis, decarboxylation and esterification give
     52% of Et α-(p-iodobenzyl)butyrate, b14 182-3°, d2020 1.415,
     n25D 1.5425.  Di-Et butyl(p-iodobenzyl)malonate, b2
     178-82°, d2020 1.362, n25D 1.5228, 67%; Et α-(p-
     iodobenzyl)caproate, b2 156°, d2020 1.352, n25D 1.5333, 68%.  Di-Et
     ethyl(3-phenylpropyl)malonate, b11 193-6°, n25D 1.4840;
     α-ethyl-δ-phenylvaleric acid, b14 189-90°, n25D 1.5033;
     iodination with NaNO2 gives 61% of an x-iodophenyl derivative, b2
     162-4°, d2020 1.362, n25D 1.5352.  The Et esters of IV and VI gave
     the most satisfactory results on intrathecal injection in dogs and by
     injection in other areas of other exptl. animals but were somewhat toxic
     in the spinal canal.  The Et ester of IV seems to be satisfactory for
     radiog. delineation of the nasal sinuses, of the Fallopian tubes and of
     various other cavities of the body.  The rate of absorption is
     sufficiently rapid so that absorption is complete in 14-18 days.
IT   1798-06-7, α-Toluic acid, p-iodo-
        (preparation of)
RN   1798-06-7  CAPLUS
CN   Benzeneacetic acid, 4-iodo- (9CI)  (CA INDEX NAME)
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